

# Different thermal conductance of the inter- and intra-chain interactions in a double-stranded molecular structure

Wei-Rong Zhong\*

*Department of Physics, College of Science and Engineering,  
Jinan University, Guangzhou 510632, P. R. China*

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## Abstract

A double-stranded system, modeled by a Frenkel-Kontorova lattice, is studied through nonequilibrium molecular dynamics simulations. We have investigated the thermal conductance influenced by the intra-chain interaction as well as by the inter-chain interaction. It is found that the intra-chain interaction always enhance the thermal conductance. The inter-chain interaction, however, has a positive effect on the thermal conductance in the case of strong nonlinear potential, and has a negative effect on the thermal conductance in the case of weak nonlinear potential. This phenomenon can be explained by the transition of thermal transport mode and the phonon band shift of the particles. It is suggested that the inter-and intra-chain interactions present different thermal properties in double-stranded lattices.

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## I. INTRODUCTION

Deriving macroscopic physics laws from simple microscopic models is one of the tasks of non-equilibrium statistical mechanics [1]. So far single-chain lattices have attracted great interest and extensive studies in the recent decades for the simple reason that they are easier to study through simulations and through whatever analytical methods are available [2] [3] [4] [5]. For one-dimensional single-chain systems, some of the most interesting results that have been obtained are as below: 1) the heat current  $J$  decreases with system size  $N$  as  $J \sim 1/N^\alpha$ , where  $\alpha < 1$  [6] [7] [8] [9]. 2) the thermal conductivity  $\kappa$  increases with the inter-particle coupling  $\lambda$  as a scaling law  $\kappa \sim \lambda^\gamma$ , here  $\gamma \sim 1.5$  [10]. In other words, the thermal conductivity is directly proportional to the interaction of the particles in single-chain systems.

In double-stranded and multi-stranded lattices, which are more common structures in nature such as DNA double helix [11], double- and multi-chain polymers [12], multi-stranded nanofibers [14] and nanotubes [13] [15], there are few detailed studies and it is fair to say that it is totally unclear as to whether they have the same properties as those the single-chain lattices have, and if not, then what they are different from. Liu and Li [16] have studied the inter-chain coupling in simple networks consisting of different one dimensional nonlinear chains. They reported that the coupling between chains has different functions in heat conduction comparing with that in electric current. However, the double-chains they have studied, which are coupled together only with two particles, are far different from the true double-stranded structure. For two dimensions nonlinear systems, which are much similar to double-stranded and multi-stranded lattices, Lee and Dhar [17] have performed simulations to determine the system size ( $L$ ) dependence of the heat current ( $J$ ). Unfortunately, the inter-and intra-chain interactions in their models have been still regarded as the same interactions.

Up to now lots of the studies about the low dimensional

thermal conductance focus on the single-chain lattices and the couplings of the particles [1], which is called the intra-chain interactions here. However, few researchers address on the influence of the inter-chain interactions on the thermal conductance. Moreover, in biological and chemical research areas, some previous investigations have shown that inter-chain interactions play an important role in the properties of materials. For instance, the inter-chain interactions can affect the denaturation of DNA [18] [19] [20] [21], the luminescent properties of polymer [22] and the electronic properties of the dimer [23]. Therefore, it is highly necessary to study the thermal properties and relevant transport problems of the inter-chain interaction. Particularly, the difference between the intra and inter-chain interaction is an important issue to be discussed.

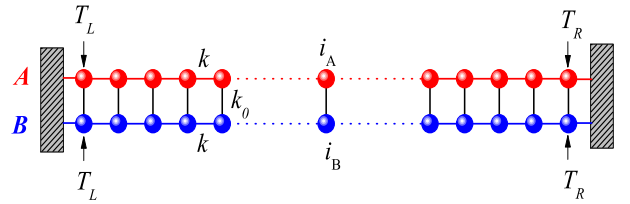


FIG. 1: Diagram of the double-stranded lattices.  $A$ -chain (red) and  $B$ -chain (blue) are coupled together via a harmonic spring  $k_0$ .  $k$  is the strength of intra-chain interaction.  $T_L$  and  $T_R$  are the temperature of the heat baths connected to the first and the last particles of each chain.

In this paper, We consider heat conduction in a double-chains Frenkel-Kontorova (FK) system as shown in Fig. 1. We expect that the inter-chain interaction can lead to some interesting and rather surprising results in thermal conductance. In this model the inter-chain interaction means the interaction between  $A$ -chain and  $B$ -chain. The intra-chain interaction, which is corresponding to the coupling of the particles in single chain system, refers to the coupling of the particles in  $A$ -chain or in  $B$ -chain. It have been reported that strong intra-chain interactions always raise the heat conductance in the single-chain FK lattice [1] [10]. A similar calculation for the inter-chain interaction is so far not available in the double-chains case, and we will address this specific question.

## II. MODEL AND SIMULATION METHOD

We consider heat conductance in a double-stranded FK crystal described by a total Hamiltonian

$$H = H_A + H_B + H_{int}. \quad (1)$$

As shown in Fig.1, we couple the  $i$ th particle of  $A$ -chain with the same order particle of  $B$ -chain via a harmonic spring, and the coupling Hamiltonian  $H_{int} = \sum_{i=1}^N [k_0 (x_{A,i} - x_{B,i})^2]$ , where  $k_0$  is the strength of the inter-chain coupling. The Hamiltonian of each chain can be written as

$$H_M = \sum_{i=1}^N \left[ \frac{p_{M,i}^2}{2m} + \frac{k}{2} (x_{M,i+1} - x_{M,i})^2 + \frac{V}{(2\pi)^2} [1 - \cos(2\pi x_{M,i})] \right], \quad (2)$$

with  $x_{M,i}$  and  $p_{M,i}$  denote the displacement from equilibrium position and the conjugate momentum of the  $i$ th particle in chain  $M$ , where  $M$  stands for  $A$  or  $B$ .  $N$  is the number of the particles in  $A$  or  $B$ -chain.  $m$  is the mass of the particle. The parameters  $V$  and  $k$  are the strength of the nonlinear external potential and the intra-chain interaction for the FK lattice, respectively. We set the masses of all the particles be unit and use fixed boundaries,  $x_{M,N+1} = x_{M,0} = 0$ . The first and the last particles of  $A$ -chain and  $B$ -chain are connected to heat baths. The temperature of the left and right heat baths is respectively  $T_L = 0.25$  and  $T_R = 0.10$ . The temperature used here and in the following numerical computations is dimensionless. It is connected with the true temperature  $T_\theta$  of the materials through the relation [24]:  $T_\theta = (m\omega_\theta^2\phi^2T)/k_B$ , here  $m$  is the mass of the particle and  $\phi$  is the period of external potential.  $\omega_\theta$  is the oscillating frequency.  $k_B$  is the Boltzmann constant.

In our simulations we use Langevin thermostat and integrate the equations of motion by using the 4th-order Runge-Kutta algorithm [25]. We chose a step size of the simulation  $\Delta t = 0.005$  and averaging over  $2 \times 10^9$  time steps. We have checked that our results do not depend on the particular thermostat realization (for example, Nose-Hoover thermostat [26]). The local temperature is defined as  $T_i = \langle p_i^2 \rangle$ ,  $\langle \rangle$  means time average. The local heat flux in double chains is defined

as  $j_i = k \langle p_{A,i} (x_{A,i} - x_{A,i-1}) \rangle + k \langle p_{B,i} (x_{B,i} - x_{B,i-1}) \rangle + k_0 \langle p_{A,i} (x_{A,i} - x_{B,i}) \rangle + k_0 \langle p_{B,i} (x_{B,i} - x_{A,i}) \rangle$ , which is derived from the equations of motion and the expression of thermal flux  $\sum (F_{M,i} \cdot v_{M,i})$ , where  $M$  stands for  $A$  and  $B$  [1]. The simulations are performed long enough to allow the system to reach a steady state in which the local heat flux is constant along the double-stranded lattice. The transport coefficient is an important quantity for characterizing the transport mode of a thermal transport process [27]. The thermal conductance evaluated as  $K = Nj/\Delta T$  represents an effective transport coefficient that includes both boundary and bulk resistances [1].

## III. RESULTS AND DISCUSSION

The inter-chain interaction is compare with the intra-chain interaction in the thermal conductance and the phonon spectra of the particles. Figure 2 shows the dependence of thermal conductance on the intra-chain interaction for the system size  $N = 64$ . For various nonlinear external potentials  $V = 1.0$  and  $10.0$  as well as two kinds of inter-chain couplings  $k_0 = 0.1$  and  $1.0$ , the thermal conductance monotonously increases with the intra-chain interaction. This result is good agreement with that of the single-chain FK lattice, which is also clearly confirmed by the analytical calculations based on the self-consistent phonon theory [10].

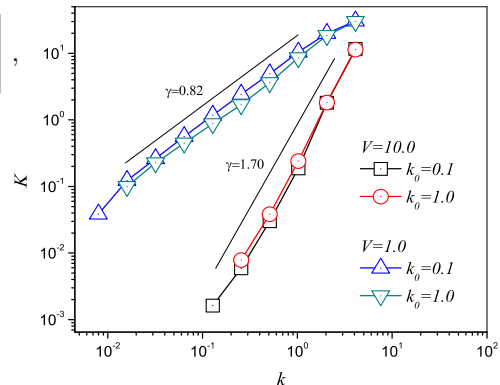


FIG. 2: Thermal conductance as a function of the intra-chain interaction for various values of  $V$  and  $k_0$  at a system size of  $N = 64$ .

Thermal conductivity dependence on  $k$  and  $V$  can be explained by the self-consistent phonon (SCP) theory. The SCP theory has been applied to deal with the nonlinear Morse on-site potential for the DNA denaturation [28]. The SCP theory can be taken into consideration the asymmetric heat transport in the nonlinearity lattices [29].

Hamiltonian of FK model can be approximated an effective linear Hamiltonian by the SCP theory as [28]

$$H = \sum_{i=1}^N \left[ \frac{p_i^2}{2m} + \frac{k}{2} (x_{i+1} - x_i)^2 + \frac{f}{2} x_i^2 \right], \quad (3)$$

where the effective harmonic potential coefficient  $f$  is obtained from the self-consistent equation,

$$f = \frac{\pi^2 V}{a^2} \exp \left[ -\frac{\pi^2 k_B T}{2a^2 \sqrt{f(4k+f)}} \right]. \quad (4)$$

So, the spectrum of effective phonons is  $\hat{\omega}_k^2 = f + 4k \sin^2 \frac{k_i}{2}$ .

As reported in Ref.[10], using Debye formula we can get the thermal conductivity as

$$K \propto \frac{ck^{3/2}}{V^2} \int_0^{2\pi} \frac{\sin^2 k_i}{(4 \sin^2 \frac{k_i}{2} + \frac{f}{k})^{3/2}} dk_i, \quad (5)$$

where  $k_i$  is the wave vector. For the sake of simplicity,  $c$  is assumed a constant, from the equation, we can obtain the relationship of  $K$  vs  $V$  and  $k$  as below:

$$K \propto \frac{k^{3/2}}{V^2}. \quad (6)$$

Thus it can be clearly seen that  $K$  increases with  $k$  as a scaling law  $K \sim k^\gamma$ , which is confirmed by numerical results as well as analytical results [10]. For single FK chain, the exponent  $\gamma$  is 3/2 and is independence of the on-site potential. However, for double FK chains, as shown in Fig.2,  $\gamma$  changes with the on-site potential  $V$  obviously. When  $V$  increases, the exponent  $\gamma$  will decreases. It can be seen that the intra-chain interaction performs a positive influence on thermal conductance not only for the single-chain lattice but also for the double-chain lattice.

When we go to the double-stranded lattice and consider the inter-chain interaction, we will find some interesting and surprising results. As shown in Fig.3, in the case of a weak nonlinear external potential  $V = 1.0$  or  $5.0$ , the thermal conductance decreases with the increasing of the inter-chain interaction. On the contrary, when the nonlinear external potential goes to a higher value  $10.0$  or  $12.0$ , the thermal conductance monotonously increase with the inter-chain interaction just as with the intra-chain interaction. Due to the universe finite size effect in low-dimensional systems, we consider more system size  $N = 256$  and  $512$ , as shown in Figs.3(b) and 3(c), the thermal conductance as a function of the inter-chain interaction mentioned above is still invariant. This indicates that this kind of anomalous heat conduction induced by the inter-chain interaction is independent of the system size.

We also like to discuss the temperature dependence of the thermal conductance. Here we set the temperature of the system as  $T_0$ . The heat baths are respectively  $T_L = T_0 + dT$  and  $T_R = T_0 - dT$ , where  $dT$  is  $0.05$ . In the case of weak on-site potential, as shown in Fig.4(a), the thermal conductance decreases with the increasing of inter-chain interaction, which is independence of the temperature. In the case of strong on-site potential, however,

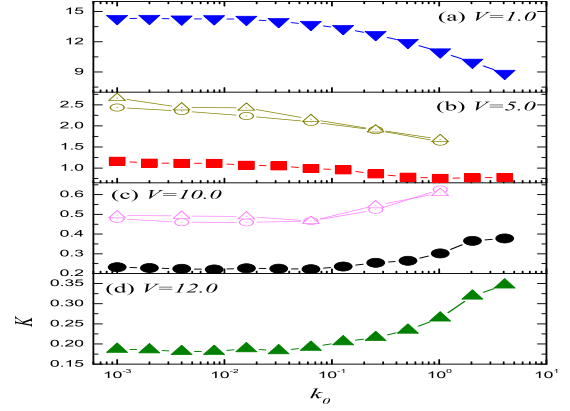


FIG. 3: The dependence of thermal conductance on inter-chain interaction for various nonlinear external potential  $V = 1.0, 5.0, 10.0$  and  $12.0$ . The system size is  $N = 64$  for full filled point ((a)blue, (b)red, (c)black and (d)green),  $256$  for circle and  $512$  for triangle ((b), (c)). The remaining parameter is  $k = 1.0$ .

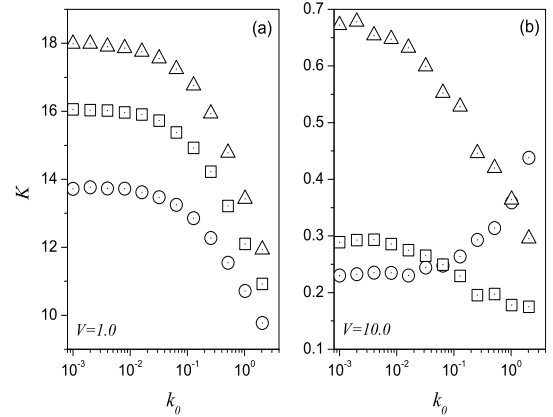


FIG. 4: Thermal conductance changes with the inter-chain interaction for various temperatures  $T_0 = 0.35$  (triangle),  $0.25$ (square),  $0.15$ (circle).

the relationship between the thermal conductance and the inter-chain interaction depends on the temperature of the system. As shown in Fig.4(b), the thermal conductance increases with the increasing of inter-chain coupling at low temperature ( $T_0 = 0.15$ ); On the contrary, the thermal conductance decreases with the increasing of inter-chain coupling at high temperature ( $T_0 = 0.25$  and  $0.35$ ).

Firstly, we apply the transition of the thermal transport mode to interpret the different thermal transport properties between intra and inter-chain interaction. For the intra-chain coupling, figures 5a and 5b show the temperature profile at different intra-chain couplings. As also

shown in the inset of Figs.5c and 5d, the thermal conductivity is finite in the diffusive region and infinite in the ballistic region. Diffusive and ballistic regions are respectively corresponding to large and small temperature differences. When the intra-chain coupling increases, the temperature difference in the chain decreases, which indicate the thermal transport mode exhibits a transition from the diffusive to the ballistic transport. Ballistic transport means less collision of phonon and then the thermal current will increase. Therefore, it is easily understood why the intra-chain coupling always enhances the thermal current in the chain. For the inter-chain coupling, as shown in Fig.5c, the inter-chain coupling cannot change the temperature profile of the chain in the case of weak nonlinear potential. However, Figure 5d displays the thermal transport mode exhibits a transition from the diffusive to the ballistic transport when inter-chain coupling increases in the case of strong nonlinear potential. The strong inter-chain interaction refers to strong on-site potential or large effective mass of the particle, which performs negative effects on the heat current. The competitive effects of strong on-site potential (negative effect) and the ballistic transport (positive effect) determine the influence of inter-chain coupling on thermal conductance. In the case of weak nonlinear potential, the transport mode is fixed and then the thermal conductance decreases with the inter-chain interaction increases. In the case of strong nonlinear potential, the on-site potential is strong enough; therefore the transition from diffusive to ballistic transport will increase the heat current.

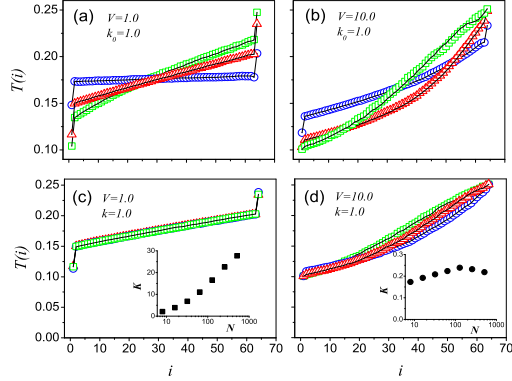


FIG. 5: Temperature profiles along A-chain (point) and B-chain (line) at various intra and interchain interactions. In (a) and (b), the parameter  $k = 0.1$  (Green square),  $0.5$  (Red triangle),  $2.0$  (Blue circle); In (c) and (d) the parameter  $k_0 = 0.01$  (Green square),  $0.1$  (Red triangle),  $1.0$  (Blue circle). Inset: the thermal conductivity changes with the system size for  $k = 1.0$  and  $k_0 = 1.0$ .

Secondly, we give another interpretation from the view of the phonon spectra. As shown in Fig.6a, when the

intra-chain interaction increases, the band width, namely the frequency range of the mid-particle of A-chain, expands. The phonon spectra of one particle can easily match the other, therefore the heat current increases. We have investigated many particles along the chain and observed similar results for other particles. However, as illustrated in Fig.6b, when the inter-chain interaction increases, the phonon spectra split into two branches when spreading. Obviously, inter-chain interaction can induce another branch of oscillation mode, which is of high oscillating frequency. The phonon is a Boson whose energy is proportion to the frequency from equation  $E = \hbar\omega$ . And then the phonon with high frequency can easily overcome the on-site potential to transmit along the chain. On the other hand, the phonon with high frequency has more opportunities to collide with each other, which means the thermal conductance decreasing. The competitive effects as mentioned above are also observed in the change of phonon spectra induced by the inter-chain interaction.

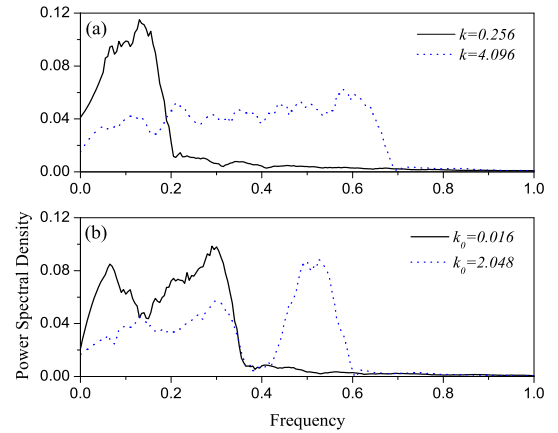


FIG. 6: Power spectral density of the particle at the middle of A-chain for different intra and interchain interaction with the parameter values  $N = 64$ ,  $V = 1.0$ , and (a)  $k_0 = 0.1$ , (b)  $k = 1.0$ .

#### IV. CONCLUSIONS

In summary, we have performed extensive numerical simulations of thermal conduction in a double-stranded FK lattice. It is reported that the interactions of the intra and inter-chain exhibit different thermal transport properties. In any case, the intra-chain interaction always upgrades the thermal conductance. The inter-chain interaction, however, has both positive and negative effects on the thermal conductance: the positive effect at the strong nonlinear potential and the negative effect at the weak nonlinear potential. Moreover, the changes of the phonon spectra of the particles, which are induced by intra-chain interaction, are quite different from those induced by inter-chain interaction. It is suggested that a simple coupling between the particles, which is a common point for both intra-chain and inter-chain interaction, can develop various thermal transport phenomena

under different situations. Although our model based on one dimensional lattice is insufficient to give a realistic description of real DNA and polymer systems, our result will provide a new physical view of DNA, polymer, nanomaterials and others structure, which are similar to double-stranded lattice.

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\* Electronic address: wrzhong@jnu.edu.cn

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